Quantum kinetic theory for the collapse of Bose-Einstein condensate

Shyamal Biswas*

Department of Theoretical Physics,

Indian Association for the Cultivation of Science,

Jadavpur, Kolkata-700032, INDIA

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We show how to apply the quantum kinetic theory in an inhomogeneous system like harmonically trapped Bose condensate. We calculate the temperature dependence of the critical number of particles by a quantum kinetic theory within the Hartree-Fock approximation and find that there is a dramatic increase in the critical number of particles as the condensation point is approached. Our results support the experimental result which was obtained well below the condensation temperature. The nature of the temperature dependence of the critical number obtained from the quantum kinetic theory is the same as obtained from the scaling theory.

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For the ultracold Bose gas, the interaction is characterized by s-wave scattering length a_s [1, 2]. Atomic interaction as well as the value of scattering length (a_s) can be controlled in Feshbach resonance[3]. Stability and collapse of Bose gas with negative scattering length has been observed in the clouds of ultracold $^7\text{Li}[4]$ and $^{85}\text{Rb}[5, 6]$. If the interaction is attractive $(a_s < 0)$, the gas tends to increase the density of the central region of the trap. This tendency is opposed by the zero-point energy and thermal energy of the atoms. If the number of atoms is greater than a critical number (N_c) , the central density increases strongly and the zero-point and thermal energy are no longer able to avoid the collapse of the gas.

To calculate the critical number (N_c) for the collapse of Bose-Einstein condensate(BEC) we do not start from the free energy but adopt a mere kinetic theory like approach based on the energy and the pressure. In the quantum kinetic theory we will start from the Hartree-Fock(H-F) energy of the system. We will pick the kinetic energy term and two body interaction term of the H-F energy. The kinetic energy of the particles causes a outward pressure and the attractive interaction causes a inward pressure. At the critical number of particles the two pressure would be the same. Beyond the critical number of particles the inward pressure would be larger than the outward pressure and the system would collapse. In this letter we shall explicitly calculate N_c by a quantum kinetic theory within the H-F approximation. We shall explicitly show the temperature dependence of N_c .

Before going into the details of the quantum kinetic theory we estimate the critical number by a semiqualitative theory. We consider a system of Bose gas of N number of particles where all the particles are harmonically trapped with angular frequency ω . Let the mass of each particles be m. As the temperature T goes to zero, all the particles come down to the ground state and the system is well described by the ground state wave function $\Psi_0(\mathbf{r}) = \sqrt{\frac{N}{l^3\pi^{3/2}}}e^{-\frac{r^2}{2l^2}}$ in the position(\mathbf{r}) space, where $l = \sqrt{\hbar/m\omega}$ is the length scale of the oscillators. For T = 0, the density of the condensed particles is described as

$$n_0(\mathbf{r}) = |\Psi_0(\mathbf{r})|^2 = \frac{N}{l^3 \pi^{3/2}} e^{-\frac{r^2}{l^2}}.$$
 (1)

In absence of collision the number density of the excited particles is [7]

$$n_T(\mathbf{r}) = \frac{1}{\lambda_T^3} g_{\frac{3}{2}} (e^{-\frac{m\omega^2 r^2}{2k_B T}}),$$
 (2)

where $\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$, and $g_{\frac{3}{2}}(x) = x + x^2/2^{3/2} + x^3/3^{3/2} + \dots$ is the Bose-Einstein function of a real variable x.

Let us consider the interaction potential as $V_{int}(\mathbf{r})=g\delta^3(\mathbf{r})$, where $g=-\frac{4\pi\hbar^2a}{m}$ is the coupling constant and $a=-a_s$ is the absolute value of the s-wave scattering length. For a dilute gas we must have $\frac{a}{l}\ll 1$. The typical two body interaction energy for N number of particles is $\sim N^2g/2l^3$. For this interaction, the gas tends to increase the density of the central region of the trap. Well below the BEC temperature(T_c), i.e. for $T\to 0$, this tendency is resisted by the zero-point energy ($\sim N\hbar\omega$) of the atoms. In the critical situation the typical oscillator energy must be comparable to the typical interaction energy. So, at T=0, we must have $N_c\hbar\omega\sim N_c^2g/2l^3$. From this relation we can write $\frac{N_ca}{l}\sim 1$.

For $0 < T < T_c$, the typical total energy of the system is [7] $N^{4/3}\hbar\omega$. So at these temperatures we must have $N_c^{4/3}\hbar\omega \sim N_c^2 g/2l^3$. From this relation we have $\frac{N_c a}{l} \sim [\frac{l}{a}]^{1/2} > 1$.

However, near T_c the length scale of the system is[7] $L_{T_c} \sim l \sqrt{\frac{k_B T_c}{\hbar \omega}} \sim l N^{1/6}$. So, near the condensation temperature we must have $N_c^{4/3} \hbar \omega \sim N_c^2 g/2 L_{T_c}^3$. From this relation we have $\frac{N_c a}{l} \sim [\frac{l}{c}]^5 \gg 1$.

^{*}Electronic address: tpsb@iacs.res.in

In the above semi qualitative argument we got $\frac{N_c a}{l} \propto 1$ for T = 0, $\frac{N_c a}{l} \propto \left[\frac{l}{a}\right]^{1/2}$ for $0 < T < T_c$ and $\frac{N_c a}{l} \propto \left[\frac{l}{a}\right]^5$ for $T = T_c$. The proportionality constants were determined by the scaling theory [8, 9]. The scaling theory gave the estimated exponents as well as the proportionality constants as [8, 9] 0.671 for T = 0, [8] $1.210 \frac{t^6}{(1-t^3)^3}$ for $0 < T < T_c$ and [8] 2.253 for $T = T_c$. Since the exponents were evaluated by a semi qualitative calculation, the evaluation of the exponents is independent of the scaling theory. It only determines the proportionality constants. In the proportionality constants there is a temperature dependence factor $(\frac{t^6}{(1-t^3)^3})$ for $0 < T < T_c$ [8]. Now we are interested to know weather this factor is independent of the scaling theory. To do so we will evaluate the proportionality constants by a quantum kinetic theory. We will see that the quantum kinetic theory will also give the correct exponents and the same temperature dependent factor of the proportionality constants. So, the scaling theory only gives the pre-factors of the proportionality constants. The quantum kinetic theory will give some different pre-factors of the proportionality

Within the H-F approximation we have the expression of energy functional as[7]

$$E = \int d^3 \mathbf{r} \left[\frac{\hbar^2}{2m} n_0 \mid \nabla \phi_0 \mid^2 + \sum_{i \neq 0} \frac{\hbar^2}{2m} n_i \mid \nabla \phi_i \mid^2 \right]$$
$$+ V(r) n_0(\mathbf{r}) + V(\mathbf{r}) n_T(\mathbf{r}) + \frac{g}{2} n_0^2(\mathbf{r})$$
$$+ 2g n_0(\mathbf{r}) n_T(\mathbf{r}) + g n_T^2(\mathbf{r}) \right]$$
(3)

To evaluate the above energy functional of eqn.(3) we have to know $n_0(\mathbf{r})$ and $n_T(\mathbf{r})$ for the interacting case. But, for the simplicity of the calculation we keep the same form of $n_0(\mathbf{r})$ and $n_T(\mathbf{r})$ as in eqn.(1) and eqn.(2). The same form of $n_T(\mathbf{r})$ is obtained from the semiclassical form of B-E statistics such that[2] $\bar{n}(\mathbf{p},\mathbf{r}) = \frac{1}{e^{(\frac{p^2}{2m} + \frac{m\omega^2r^2}{2})/k_BT}}$, where \mathbf{p} is the momentum of a single particle. With this form of statistics we have the total number of excited particles as $N = (\frac{k_BT_c}{\hbar\omega})^3\zeta(3)$. For $T \leq T_c$, the total number of particles in the ground state is $n_0 = N - N_T = N(1 - \frac{T}{T_c})^3$. From the variation in statistics we evaluate the energy functional of eqn.(3) as

$$E(t) = [(1+1)c_1(t) - c_2]N \frac{\hbar^2}{ml^2}$$
(4)

where
$$t = T/T_c$$
, $c_1(t) = \frac{3}{4}(1-t^3) + \frac{3}{2}\frac{N^{1/3}\zeta(4)t^4}{[\zeta(3)]^{4/3}}$ and $c_2(t) = \frac{1}{\sqrt{2\pi}}\frac{Na}{l}[1-t^3]^2 + \sqrt{\frac{8\zeta(3/2)}{\pi}}\frac{N^{1/2}a}{l}t^{3/2}[1-t^3] + S'\sqrt{\frac{2}{\pi[\zeta(3)]^3}}\frac{N^{1/2}a}{l}t^{9/2}$ such that $S' = \sum_{i,j=1}^{\infty}\frac{1}{(ij)^{3/2}(i+j)^{3/2}}\approx 0.6534$.

From the above eqn.(4) we get the kinetic energy of

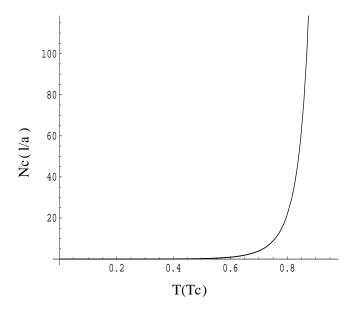


FIG. 1: Plot of the critical number N_c in units of $\frac{l}{a}$ with temperature(T) in units of (T_c). Here $\frac{l}{a} = 0.0066$ [6]. This plot follows form eqn.(9).

the system as

$$E_k(t) = c_1(t)N\frac{\hbar^2}{ml^2} \tag{5}$$

and get the interaction energy of the system as

$$E_{int}(t) = c_2(t)N\frac{\hbar^2}{ml^2} = -c_3(t)N^2a\frac{\hbar^2}{ml^3}$$
 (6)

where
$$c_3(t) = \frac{1}{\sqrt{2\pi}} [1 - t^3]^2 + \sqrt{\frac{8\zeta(3/2)}{\pi}} N^{-1/2} t^{3/2} [1 - t^3] + S' \sqrt{\frac{2}{\pi [\zeta(3)]^3}} N^{-1/2} t^{9/2}.$$

For $0 \le T < T_c$, the effective volume of the system is $V = 4\pi l^3/3$. The outward pressure is $P_{out} = -\frac{\partial E_k}{\partial V}$. The magnitude of the inward pressure is $P_{in} = \frac{\partial E_{int}}{\partial V}$. At the critical number of particles P_{in} would be equal to P_{out} . From this equality relation we can write the expression of the critical number as

$$N_c = \frac{2c_1(t)}{3ac_3(t)} \left(\frac{3V}{4\pi}\right)^{1/3} \tag{7}$$

Eqn.(7) gives the expression of the critical number as

$$\frac{N_c a}{l} = \frac{2c_1(0)}{3c_3(0)} = \sqrt{\frac{\pi}{2}} = 1.253 \text{ for } T = 0.$$
 (8)

Now we see that our scaling result with $T \geq 0$ is consistent with the scaling result of [8, 9] for T=0. The numerical result for T=0 is [10] $\frac{N_c a}{l}=0.575$ and the experimental result for T=0 is [6] $\frac{N_c a}{l}=0.459$.

To achieve the Bose-Einstein statistics the necessary condition is such that [7] $a/l \ll 1$. For $0 < T \le T_c$, considering $a/l \ll 1$, we can approximately write $c_1(t) =$

 $\frac{3}{2}\frac{N^{1/3}\zeta(4)t^4}{[\zeta(3)]^{4/3}}.$ Similarly, for $0 < T \le T_c$, we can approximately write $c_3(t) = \frac{1}{\sqrt{2\pi}}[1-t^3]^2.$ For $0 < T < T_c$, the expression of N_c obtained from eqn.(7) is $\frac{N_c a}{l} = \frac{2\times\frac{3}{2}\frac{N_c^{1/3}\zeta(4)t^4}{[\zeta(3)]^{4/3}}}{3\frac{1}{\sqrt{2\pi}}[1-t^3]^2}.$ From this relation we can write

$$\frac{N_c a}{l} = 0.779 \left[\frac{l}{a}\right]^{1/2} \frac{t^6}{(1 - t^3)^3} \quad for \quad 0 < T < T_c.$$
 (9)

The above eqn.(9) is represented in FIG. 1. Now we see that the nature of the temperature dependence of the critical number is the same as obtained from the scaling theory[8].

For $T=T_c$, the length scale of the system is [7] $L_{T_c}=lN^{1/6}$. For this case the effective volume of the system is $V=4\pi l^3N^{1/2}/3$. For this reason the critical condition would be the same as eqn.(7) except the factor V which is to be replaced by $\frac{V}{N_c^{1/2}}$. So, for $T=T_c$ the expression of N_c would be obtained from

$$N_c = \frac{2c_1(1)}{3ac_3(1)} \left(\frac{3V}{4\pi N_c^{1/2}}\right)^{1/3}.$$
 (10)

Putting the value of $c_1(1)$ and $c_3(1)$ into the eqn.(10) we get

$$\frac{N_c a}{l} = 96.062 \left[\frac{l}{a}\right]^5 \quad for \quad T = T_c$$
 (11)

Now we see that the critical number increases dramatically as the condensation point is approached.

Initially we qualitatively explained the physics of the collapse of the attractive atomic Bose gas. Then we semi qualitatively estimated $N_c a/l$ for the various range of temperatures $(0 \le T \le T_c)$. Finally we calculate $N_c a/l$ by a quantum kinetic theory within the Hartree-Fock approximation. Our calculation supports the semi qualitative estimation of $N_c a/l$. The quantum kinetic theory gives the same nature of the temperature dependence of the critical number as obtained from the scaling theory. Since $\frac{l}{a}$ is a very large number and the nature of the temperature dependence of the critical number is the same for the two different theories, the two theories are equal a priory and self consistent with respect to the basic physics of the collapse of the Bose gas. However, the calculations of the scaling theory is more rigorous than that of the quantum kinetic theory. The scaling theory result at T=0 is also closer to the experimental result.

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